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5,6-Dihydroxy-7-methoxyflavone

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C(17)	0.0951 (2)	0.2629 (4)	−0.1866 (2)	0.0441 (13)
C(18)	0.0076 (3)	0.3419 (5)	−0.0336 (3)	0.0514 (16)
C(19)	0.0023 (3)	0.3431 (6)	0.0826 (3)	0.0590 (17)
C(20)	0.1364 (2)	0.2839 (4)	0.1491 (2)	0.0412 (13)
C(21)	0.1965 (3)	0.4623 (4)	0.3742 (2)	0.0445 (14)
C(22)	0.3322 (3)	0.5198 (5)	0.4718 (3)	0.0480 (15)
C(23)	0.1488 (3)	0.6812 (5)	0.5157 (3)	0.0548 (16)
C(24)	0.2276 (4)	0.7864 (5)	0.4611 (3)	0.0621 (21)
C(25)	0.2940 (4)	0.7331 (5)	0.3644 (3)	0.0593 (22)
C(26)	0.2798 (4)	0.5684 (5)	0.3321 (3)	0.0520 (21)

Table 2. *Selected geometric parameters* (Å, °)

P—C(1)	1.833 (3)	P—C(20)	1.819 (2)
P—C(21)	1.835 (3)	C(1)—C(10)	1.391 (4)
C(10)—C(11)	1.479 (4)	C(11)—C(20)	1.391 (4)
H(8)···H(13)	2.33 (5)		
P—C(1)—C(2)	125.7 (2)	P—C(1)—C(10)	112.5 (1)
P—C(20)—C(11)	111.8 (2)	P—C(20)—C(19)	125.9 (2)
P—C(21)—C(22)	119.6 (2)	P—C(21)—C(26)	121.7 (3)
C(1)—P—C(20)	89.6 (1)	C(1)—P—C(21)	100.9 (1)
C(20)—P—C(21)	103.2 (1)	C(2)—C(1)—C(10)	121.8 (3)
C(1)—C(10)—C(9)	117.9 (2)	C(1)—C(10)—C(11)	112.2 (2)
C(9)—C(10)—C(11)	129.6 (2)	C(10)—C(11)—C(12)	129.1 (3)
C(10)—C(11)—C(20)	112.6 (2)	C(12)—C(11)—C(20)	118.1 (2)

Table 3. *Dihedral angles (°) between least-squares planes*

Plane 1: P, C(1), C(10), C(11), C(20). Plane 2: C(1)–C(4), C(9), C(10). Plane 3: C(4)–C(9). Plane 4: C(11), C(12), C(17)–C(20). Plane 5: C(12)–C(17). Plane 6: C(21)–C(26). Napl 1: C(1)–C(10). Napl 2: C(11)–C(20).

Plane 1—Plane 2	6.07 (9)	Plane 1—Plane 4	12.03 (9)
Plane 1—Plane 6	90.9 (2)	Plane 2—Plane 3	12.2 (2)
Plane 2—Plane 4	18.3 (2)	Plane 3—Plane 5	38.2 (2)
Plane 4—Plane 5	9.6 (1)	Napl 1—Napl 2	28.7 (1)

The positional parameters for all non-H atoms were determined by direct methods (Sheldrick, 1985). The refinements were carried out by full-matrix least-squares techniques (Imoto, 1990). All H atoms were located in a difference Fourier map. The $\Delta f'$ and $\Delta f''$ components of anomalous dispersion were included in the calculation for the P atom (Cromer & Ibers, 1974). The refined structure showed *P* helicity. On the other hand, the enantiomeric structure gave *R* and *wR* values of 0.0494 and 0.0601. Thus, we decided that the title compound has the absolute configuration *P*. All calculations were carried out on an NEC ACOS 930S computer at the Research Center for Protein Engineering, Institute for Protein Research, Osaka University.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71696 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1077]

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5,6-Dihydroxy-7-methoxyflavone

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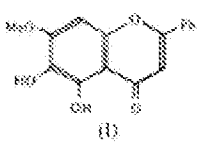
Abstract

The 5-hydroxy group of the title compound, 5,6-dihydroxy-7-methoxy-2-phenyl-4*H*-1-benzopyran-4-one, $C_{16}H_{12}O_5$, forms a cyclic intramolecular hydrogen bond O(3)—H···O(2), H···O = 1.71 (3) Å, with the carbonyl group. The heterocyclic ring is not coplanar with the phenyl ring. The C(7) methoxy group is in the plane of the γ-benzopyrone ring with the torsion angle C(11)—O(4)—C(7)—C(8) = 2.9 (3)°.

Comment

The dihedral angle of 12.2 (2)° between the phenyl ring and the γ-benzopyrone portion of the molecule (I) is significantly different from those of two related structures, 5-hydroxy-7-methoxyflavone (Shoja, 1989) and 5-hydroxyflavone (Shoja, 1990), with dihedral angles of 24.8 (2) and 5.7 (7)°, respectively. Given the wide range of dihedral angles and the fact that all three of these molecules contain hydrogen bonding, it is unlikely that any planarity is solely a



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